Nano Vision, Vol.1 (1), 25-33 (2011)

Variation of Electronic State of CUBOID Quantum Dot with Size

RAMA SHANKER YADAV and B. S. BHADORIA*

Department of Physics, Bundelkhand University, Jhansi-284128 U.P. India
email: ramaphysics09@gmail.com

ABSTRACT

Quantum dot structures are 3D confinement nano structures which involve the formation of excitons (electron & hole pair) which result the discrete density of states to represent the atom like behavior. This paper involves the CUBOID shape of quantum dot in which the infinite confinement potential is used to calculate the energy levels of electrons and holes and does not involve the potential due to piezoelectricity, coulombic interaction and stress distribution in quantum dot. The energy levels are variable when the base, height, volume and aspect ratio are changed. The paper represents the variation of ground state energy with these parameters. It also represents the non monotonic energy variation due to aspect ratio. The most important tunable property of quantum dot is the blue shift of material. This paper also represents the amount of the blue shift due to variation of base, height and volume of CUBOID quantum dot. Quantum dot is the material for advanced research. This study will provide a better way to experimentalist to choose the material dimensions according to their practical use.

Keywords: Aspect Ratio, Blue Shift, Density of States.

1. INTRODUCTION

Semiconductor nanostructures confine electron and hole excitations in small regions that extend from several to hundreds of nanometers. There are many reasons to develop nanostructures, such as their ability to enhance optical absorption and emission, the continuing miniaturization of digital circuitry, and the study of few-body quantum phenomenon and possible exploitation for quantum computation[1]. Semiconductor research and development has seen progressive reduction in dimension, from bulk material to quantum well, and then to quantum wire, and eventually to quantum dot (QD).

The quantum dots are 3D confinement nano structures with enhanced optical and electronic study. In a quantum dot the single particle energies of electrons or holes depend almost solely on the quantum dots structural properties like size, shape, composition and the surrounding material. These desired properties of quantum dots have spun new research in various QD devices, e.g., laser, infrared photo detector (QDIP), and electro absorption modulator (EAM)[2]. However, as there are specific requirements for different QD devices, there is a need to alter the dimensions of the active material to suit the requirements.

The energy difference between ground-state energy and excited-state energy is important for carrier dynamics e.g., relaxation time for laser and escape time for detector, and is of great concern for high speed device operation[2]. In practice, the QD shape and size will exert a significant influence on its electronic structure, optical property and hence wavelength characteristic.

This paper presents our work on the electronic states of InAs/GaAs CUBOID quantum dot and the effect of size variation. Our study aims to understand the energy trends of CUBOID QD as a function base, height, volume and aspect ratio, in order to obtain the energy dependency on each QD dimension variation.

2. MODEL

The cross-sectional and plan views of CUBOID quantum dot shape with boundary conditions are shown in figure 1. Note that cubic is a special case of CUBOID (i.e., when $h=b$).

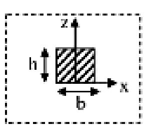
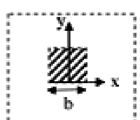
QD shape Cross section	QD shape Plan view	Name (Abbreviation)	Boundary definition and volume
		Cuboid QD (CUBOID)	$\lvert x\rvert \le b/2$ $\lvert y\rvert \le b/2$ $0 \le z \le h$ $V_{CUBOID}=hb^2$

Figure-: 1 ***Cross section and Plane view of CUBOID quantum dot.***

Table 1 illustrates the physical parameters considered in this study, namely, the volume (Vol), base length (*b*), height (*h*), and aspect ratio (AR). As QD volume is varied, aspect ratio of all QD shapes is fixed at 0.5 (i.e., AR=0.5), so that the height-to-base ratio is kept constant throughout.

Table- 1 Physical Parameter for Quantum Dot

Parameter	Aberrations	Parameter range(Å)
QD Base	b	50-400
QD Height	h	20-140
QD Volume	vol	10^4-10^7
QD Aspect ratio	AR	0.2- 2.0

In order to study the variation of size on CUBOID quantum dot, the range of volume variation (from 10^4 to 10^7 $Å^3$) is considered realistic, as these translate to a base of (50 Å) and height (25 Å) to a base of (400 Å) and height of (200 Å), respectively[3,4]. To

study the base and height variation, the QD height was maintained at 100 Å as the base length is varied. This is to isolate the effect of height and focus on the impact of base length variation on the energy states. Likewise, for the case of height variation, the base length was fixed at 200 Å as the height is varied, so as to isolate the effect of base and focus on the impact due to height variation.

To investigate the effect of QD aspect ratio (AR) variation, the volume of Cuboid QD shape was fixed at 1000 nm^3.This will allow us to focus on the effect of AR changes on the energy states as the volume is held constant[5]. The bound state energies increase following increase in confinement.

The single-band effective-mass approximation to Schrödinger's equation has been used to calculate the electron and heavy-hole energy levels. Within the framework of the envelope function and effective mass theory, the Hamiltonian can be written as

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + V(r)$$

$$V(r) = \begin{cases} 0 & \text{in quantum dot} \\ \infty & \text{outside the dot} \end{cases}$$

Where m* is the effective mass of carriers in semiconductor materials[2]. The wave functions are expanded in terms of normalized plane waves, where L_x, L_y, L_z are lengths of the unit cell along the *x*, *y*, and *z* directions, respectively; n_x, n_y, n_z are the number of plane waves along the *x*, *y*, and *z* directions, respectively; $k_{nx}= k_x+n_xK_x$, $K_x=2\pi/L_x$; $k_{ny}=k_y+n_yK_y$, $K_y=2\pi/L_y$; and $k_{nz}=k_z+n_zK_z$, $K_z=2\pi/L_z$.

$$\psi(x,y,z) = \frac{1}{\sqrt{L_xL_yL_z}}\sum_{nx,ny,nz} a_{nx,ny,nz}e^{i(k_{nx}x+k_{ny}y+k_{nz}z)}$$

The electron and hole energy states were calculated using the discretized Schrödinger's equation technique. Seven normalized plane waves in each direction were used to form the Hamiltonian matrix, i.e., with n_x, n_y, n_z each ranging from −3 to 3. Hence, a 343×343 matrix is formed, and the energy eigenvalues and eigenfunctions can be solved using relatively modest computing resources[2]. We have also ignored additional effects, such as potential due to piezoelectricity, Coulombic interaction, and strain distribution within the QD. The effect of piezoelectric potential is ignored since its effect on the energy levels involved in optical transitions is only marginal (1 meV)[6]. Furthermore, the QDs considered in this paper are within the strong confinement regime, i.e., the effective radius is much smaller compared to the bulk exciton Bohr radius. Therefore, Coulombic interaction effects can be ignored[7].

3. RESULT & DISCUSSION

This section discusses the results and physics behind the Observed trends as the physical parameters are varied. The increase in the QD volume, base length, or height results in decrease in the energy states due to reduction in the confinement effect. The material used in this theoretical study is InAs with the character of energy band gap 0.720eV, electron effective mass $0.04m_o$ and hole effective mass $0.59m_o$. The electron ground-state energies of CUBOID QD shapes, as function of QD volume, are shown in Fig.2 (a), while the heavy-hole

ground-state energies are shown in Fig. 2(b). In this case, all the CUBOID QD shapes have a fixed aspect ratio of 0.5. The calculated energy is dependent on volume as $E \sim V^{-Y}$ with Y =2/3 for the CUBOID QD with infinite barrier.

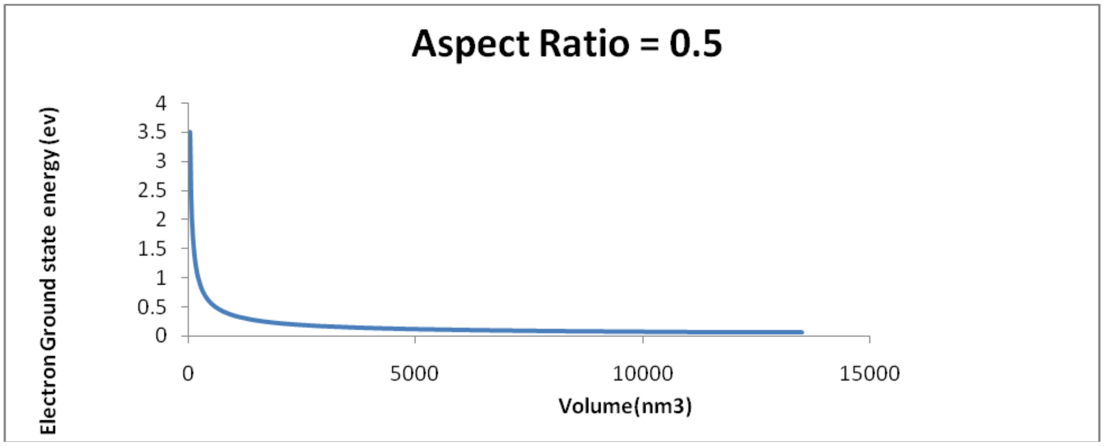


Figure-:2(a) Variation of Electron's Ground state Energy wrt Volume for InAs cuboid QD

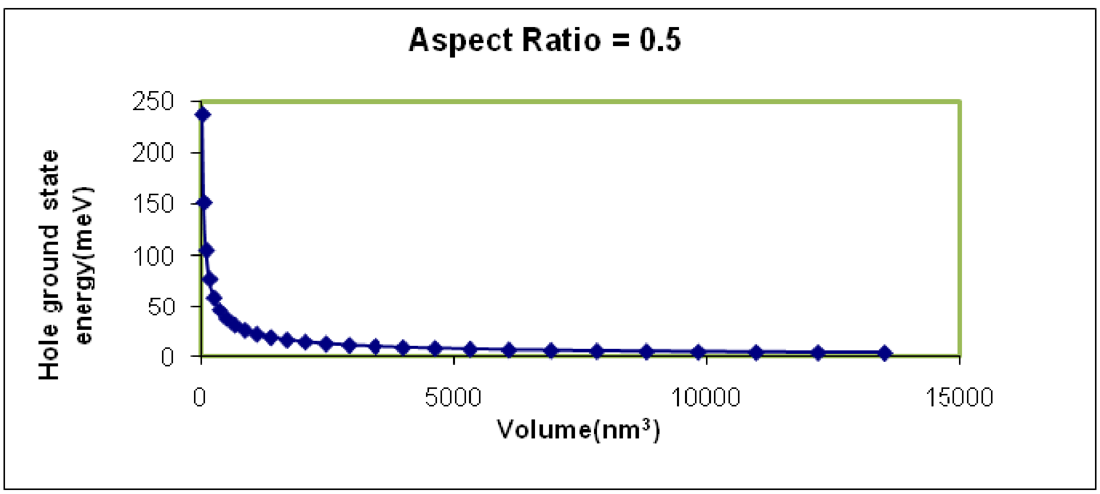


Figure-:2(b) Variation of Hole's Ground state Energy wrt Volume for InAs cuboid QD

The volume dependency Y^{Vol} And base length (height) dependency $Y^{b}(Y^{h})$ are significantly different; i.e., while Y^{Vol}= 0.67, Y^{b}=Y^{h}=2. This significant difference in the dependency can be used as a means to understand the QD formation process, i.e., whether addition of InAs coverage will result in increase of the volume or height (base length) of the QD. The variation of carriers ground state energy with base and height is shown in figure 3(a),3(b),4(a) and 4(b). The energy dependencies are significantly different, i.e., Y^{Vol}. is approximately three times smaller than Y^{h}

(or Y^b). This large difference can be very useful for verification of QD formation.

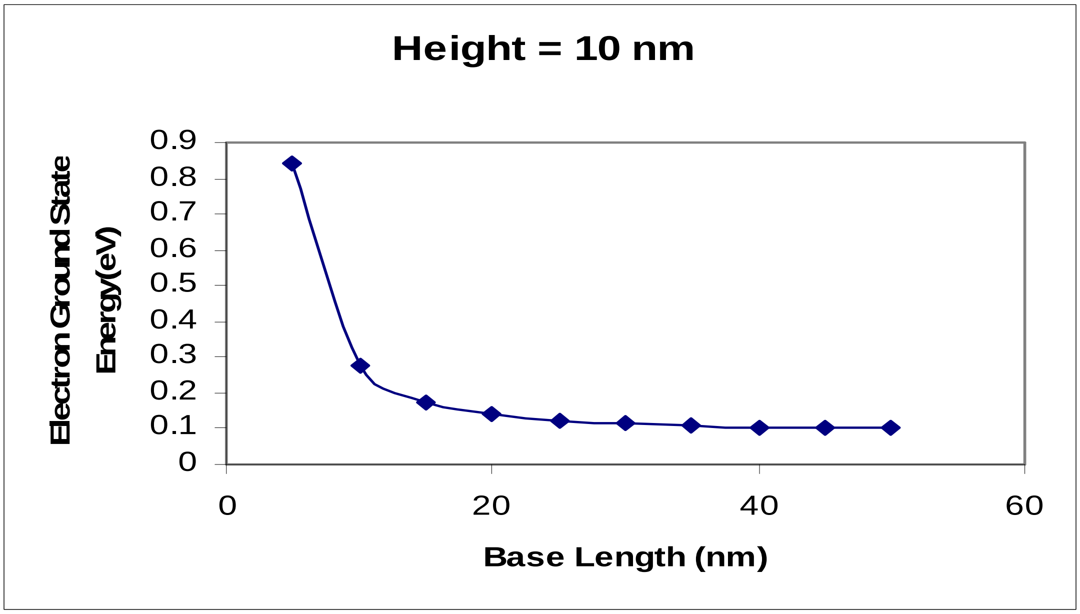


Figure-: 3(a) Variation of Electron's Ground State Energy wrt Base for InAs Cuboid QD

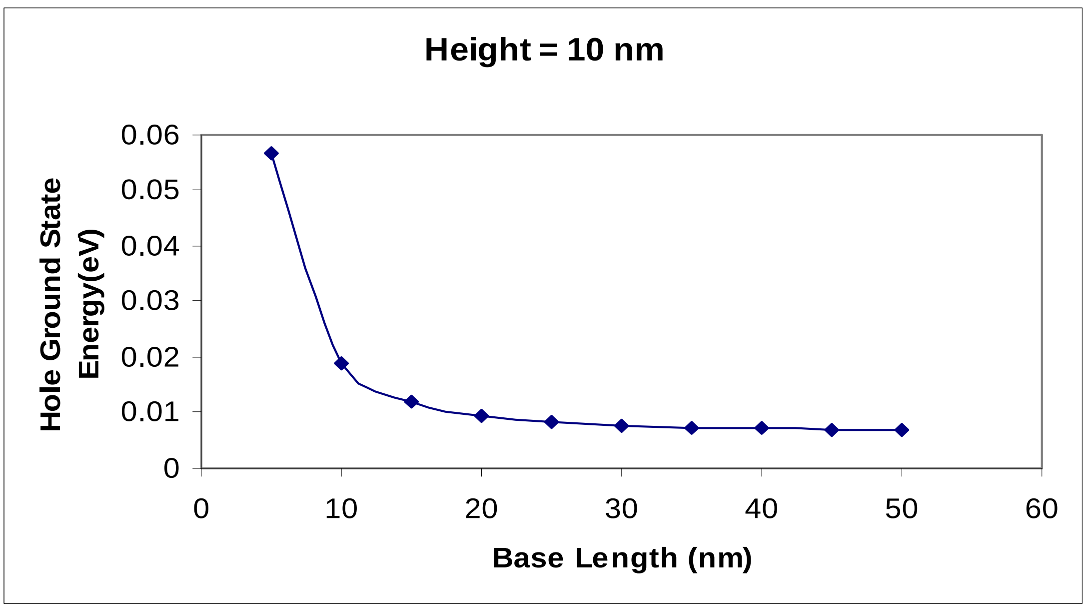


Figure-:3(b) Variation of Hole's Ground State Energy wrt Base for InAs Cuboid QD

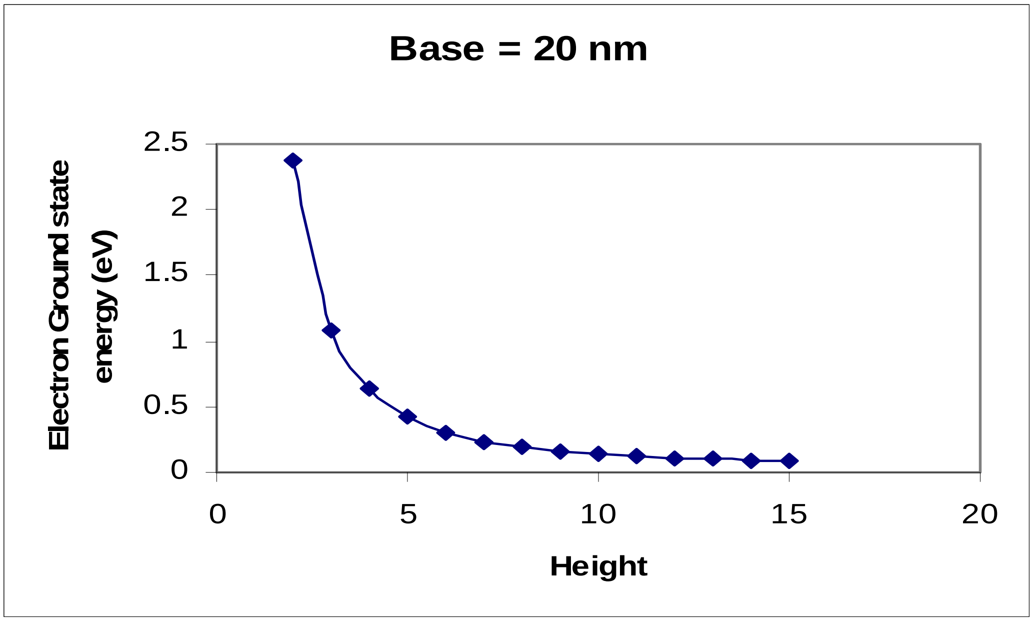


Figure-:4(a) Variation of Electron's Ground state Energy wrt Height for InAs cuboid QD

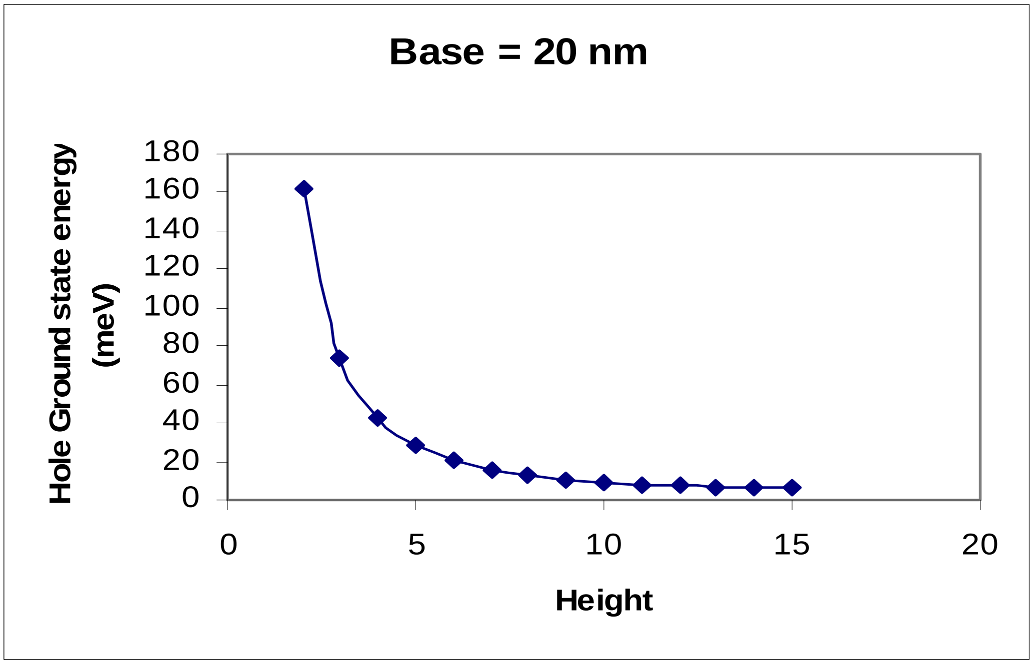


Figure-:4(b) Variation of Hole's Ground state Energy wrt Height for InAs cuboid QD

Our calculated results of energy states as function of aspect ratio for fixed volume 1000nm^3 CUBOID QD shapes are shown in Figure 5(a) and 5(b). The energy states do not follow monotonic trends. Instead, there is an “optimum” aspect ratio for each QD shape where the energy state is the lowest.

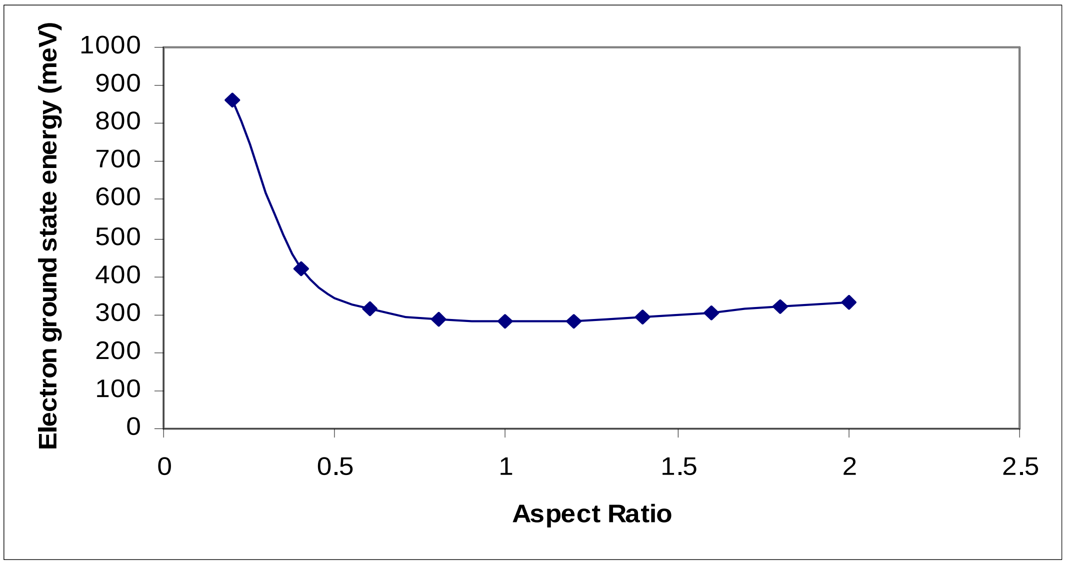


Figure-:5(a) Variation of Electron Ground state Energy wrt Aspect ratio for InAs cuboid QD

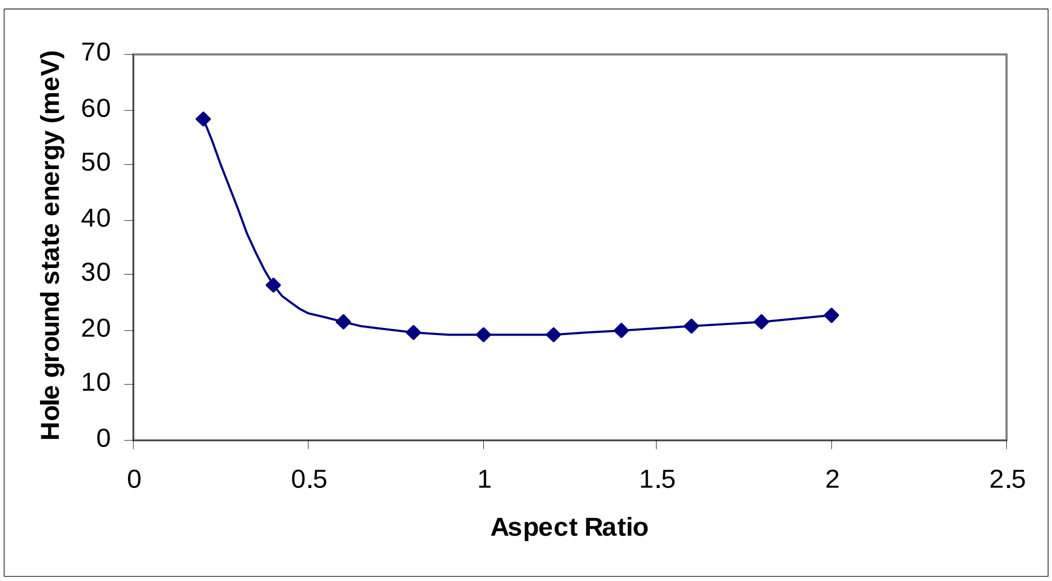


Figure-:5(b) Variation of Hole Ground state Energy wrt Aspect ratio for InAs cuboid QD

It is seen that the energy state exhibits two different trends: a steep decrease ($AR^{-4/3}$) for smaller aspect ratio followed by a gentle, almost linear increase ($AR^{2/3}$). We consider the competing effects of decrease in base length and increase in height, as aspect ratio increases. For smaller aspect ratio, decrease in confinement energy due to increase in height is much larger than increase in confinement energy due to decrease in base length. This explains the steep decrease in the ground-state energy following a small increase in aspect ratio. The inverse is also true for large increase in aspect ratio.

The reduction of size on the semiconductor material results in the variation in it's properties as optical band gap, conductivity etc. Due the reduction in size, the optical band gap increases because the confinement increases which results in higher energy exciton. Such variation in optical band gap is shown in figure 6.

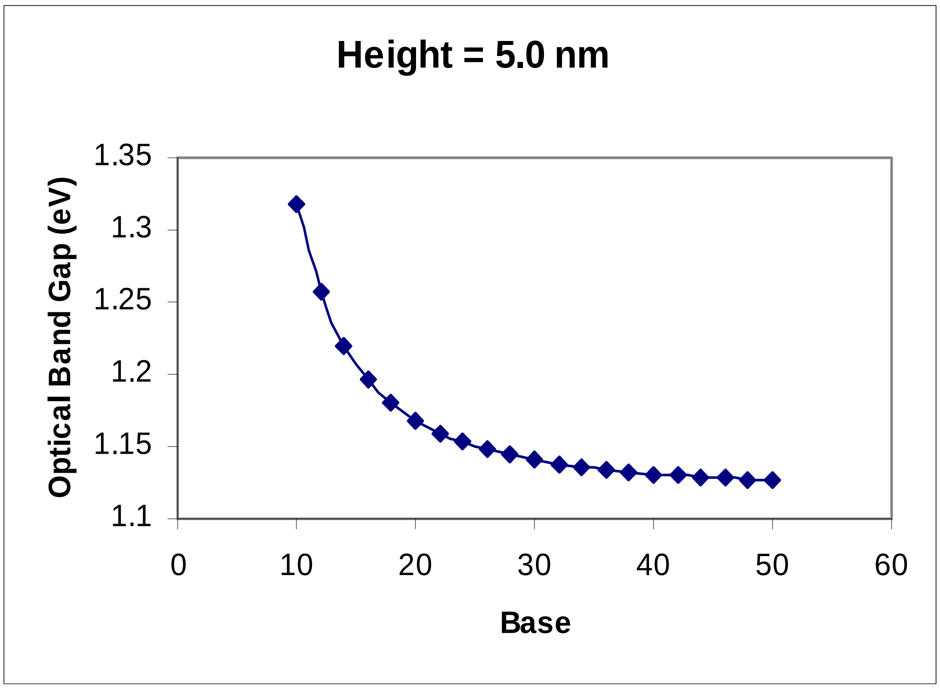


Figure-:6 Variation of optical band gap wrt Base for cuboid QD

It results that the variation of 1nm in base length results 3.6meV blue shift and variation of 1nm in height results 121.9meV blue shift for the cuboid quantum dot of InAs semiconductor material[8]. It results that vertical confinement is more effective than horizontal confinement.

4. CONCLUSIONS

This paper reports single-band, constant-potential three-dimensional model to study the dependence of electronic states of InAs CUBIOD quantum dots (QDs) of different sizes. Our calculations were found

to be consistent with experimental results and atomistic calculations from current literature. This study represents that energy of electrons and holes has the monotonic decreasing nature on increasing the quantum dot size. The energy dependency is approximately three times larger for volume variation in comparison to height (base) variation. It also results the blue shift in the InAs semiconductor material due to base and height variation. Another representation is the non monotonic energy trends for the variation of aspect ratio of the quantum dot.

5. REFERENCES

1. Matthew Harowitz, Daejin Shin, and John Shumway, *Journal of low tem. Physics, Vol. 140* (2005).
2. C. Y. Ngo, S. F. Yoon, and W. J. Fan, *Phys. Rev. B.*74.245331 (2006).
3. Gunawan, H. S. Djie, and B. S. Ooi, Phys. Rev. B 71, 205319 (2005).
4. S. S. Li, J. B. Xia, Z. L. Yuan, Z. Y. Xu, W. Ge, X. R. Wang, Y. Wang, J. Wang, and L. L. Chang, *Phys. Rev. B* 54, 11575 (1996).
5. R. V. N. Melnik and K. N. Zotsenko, Modell. Simul. *Mater. Sci. Eng.* 12, 465 (2004).
6. M. Grundmann, O. Stier, and D. Bimberg, *Phys. Rev. B* 52, 11969 (1995).
7. D. Bimberg, M. Grundmann, and N. N. Ledentsov, *Quantum Dot, Hetero-structures*, (Wiley,Chichester, 1999).
8. M Usman *et al*., IEEE Transaction of Nanotechnology, (2009).